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Direct absorption IR, LIF, REMPI and velocity map imaging methods developed under AFOSR support have been used to study state-to-state inelastic and reactive scattering dynamics under single collision conditions. Efforts over this past year have led to progress in multiple areas: 1) Diode laser and LIF studies of hyperthermal CO2 and NO collisions at the gas-room temperature ionic liquid (RTIL) interfaces. 2) Large scale trajectory simulations for theoretical analysis of gas-liquid scattering studies, 3) LIF data for state-resolved scattering of hyperthermal NO at the gas-molten Ga(l) interface as a function of incident energy and surface temperature, 4) Velocity map ion imaging studies elucidating state-resolved reactive scattering dynamics of HCl from self assembled monolayers (SAMs). 5) Ultrafast plasmon mediated electron ejection dynamics in single Au nanostructures via novel scanning photo-ionization imaging microscopy (SPIM) methods developed in our group.

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State-to-state thermal/hyperthermal collision dynamics of atmospheric species

Abstract:

Direct absorption IR, LIF, REMPI and velocity map imaging methods developed under AFOSR support have been used to study state-to-state inelastic and reactive scattering dynamics under single collision conditions. Efforts over this past year have led to progress in multiple areas: 1) Diode laser and LIF studies of hyperthermal CO2 and NO collisions at the gas-room temperature ionic liquid (RTIL) interfaces. 2) Large scale trajectory simulations for theoretical analysis of gas-liquid scattering studies, 3) LIF data for state-resolved scattering of hyperthermal NO at the gas-molten Ga(l) interface as a function of incident energy and surface temperature, 4) Velocity map ion imaging studies elucidating state-resolved reactive scattering dynamics of HCl from self assembled monolayers (SAMs). 5) Ultrafast plasmon mediated electron ejection dynamics in single Au nanostructures via novel scanning photo-ionization imaging microscopy (SPIM) methods developed in our group.

Summary of research accomplishments (2008-present)

The current granting period has been highly productive; over the last three years, 23 manuscripts from our group have been published on AFOSR-supported projects, with selected highlights summarized below.

A. Surface Temperature Dependent Collision Dynamics at Gas-Liquid Interfaces

As a major thrust over the last granting period, we have refined the technology for quantum state resolved scattering at the gas-liquid interface to an unprecedented level of absorbance sensitivity, which has enabled a number of studies.[1-7] For example, energy transfer dynamics at the gas-liquid interface has been investigated as a function of surface temperature (Fig. 1) both by experimental studies of CO_2 + perfluorinated polyether (PFPE) and molecular dynamics simulations of CO_2 + fluorinated self-assembled monolayers (F-SAMs).[6] At *low* incident energies [E_{inc} = 1.6(1) kcal/mol], CO_2 J-state populations and transverse Doppler velocity distributions are in quantitative agreement with the surface temperature ($T_{rot} \approx T_{trans} \approx T_S$) over the range from 230K – 320K. In contrast, the rotational and translational distributions at *high* incident energies [E_{inc} = 10.6(8) kcal/mol] show evidence for both trapping-desorption (TD) and impulsive scattering (IS) events. Nevertheless, the populations are surprisingly well characterized by a sum of Boltzmann distributions where one component (TD) is equilibrated with the surface ($T_{TD} \approx T_S$), while the second (IS) is much hotter than the surface temperature ($T_{IS} >> T_S$). Support for the superthermal, yet Boltzmann, nature of the IS channel is provided by molecular dynamics (MD) simulations of CO_2 + F-SAMs [E_{inc} = 10.6 kcal/mol], which also reveal dual-temperature distributions, sticking probabilities, and angular distributions in remarkably quantitative agreement with the experimental PFPE results. Interestingly, experiments as a function of surface temperature reveal an *increase* in both sticking probability as well as rotational/translational temperature of the IS component. Such a trend is consistent with increased surface roughness at higher surface temperatures,[8] which increases the overall probability of trapping, yet also preferentially leads to greater torque to yield more highly rotationally excited CO_2 recoiling impulsively from the surface.

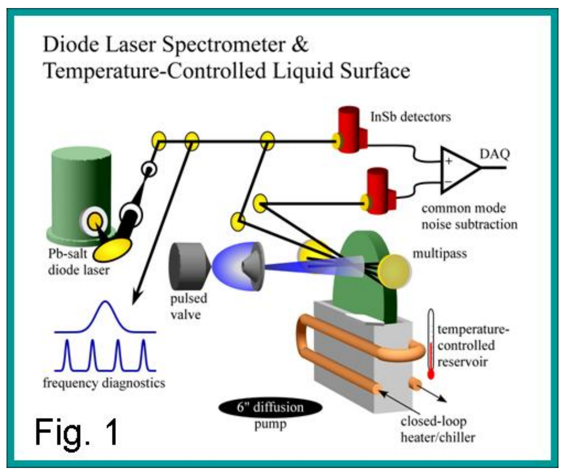


Fig. 1

B. Incident and Final Angle Resolved Collision Dynamics at the Gas-Liquid Interface

Quantum state resolved detection by direct IR laser absorption in a tight optical multipass offers exceptional flexibility and control over incident and probe geometries, which can be exploited to probe scattering into a full 2π solid angle. For example, molecular beam scattering dynamics at the gas-liquid interface has been investigated for CO_2 (E_{inc} = 10.6(8) kcal/mol) impinging on liquid PFPE, with quantum-state (v, *J*) populations measured as a function of incident (θ_{inc}), and final (θ_{scat}) scattering angles (Fig. 2).[9] The internal state distributions are well-characterized for both normal and grazing incident angles by a two-component Boltzmann model for trapping desorption (TD) and impulsive scattering (IS) at rotational temperatures T_{rot}(TD/IS). The angular dependence of the IS flux at normal incidence ($\theta_{inc} = 0°$) is surprisingly well modeled by a simple $\cos^n(\theta_{scat})$ distribution with $n = 1.0 \pm 0.2$, while glancing incident angles (θ_{inc} = 30°, 45°, and 60°) result in lobular angular IS distributions scattered preferentially in the forward direction. This trend is also corroborated in the TD fraction α, which *decreases* rapidly under non-normal incident conditions as a function of backward versus forward scattering direction. Furthermore, the extent of rotational excitation in the IS channel *increases* dramatically with angle of incidence, consistent with an *increasing* rotational torque sampled by the projectile by virtue of molecular scale roughness at the gas-liquid interface.

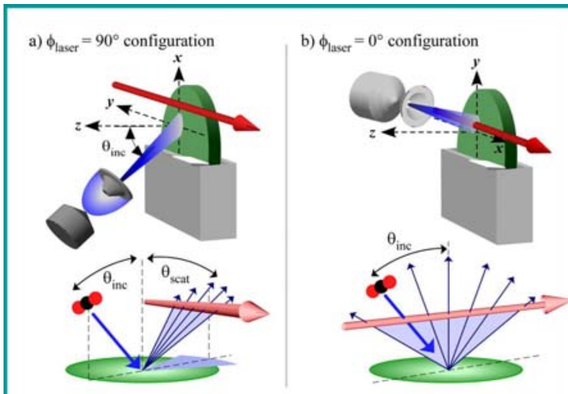


Fig. 2

C. Reaction Dynamics at the Gas–Liquid Interface: F + Squalane ($C_{30}H_{62}$)

One powerful direction has been to use direct infrared laser absorption spectroscopy to probe fast chemical reactions by colliding a supersonic beam of F atoms [E_{com} = 0.7(3) kcal/mol] with a continuously refreshed liquid hydrocarbon (squalane) surface under vacuum conditions (Fig. 3).[7] Nascent HF($v \le 3$) products are formed in a highly non-equilibrium (inverted) vibrational distribution [$\langle E_{vib} \rangle$ = 13.2(2) kcal/mol], reflecting insufficient time for complete thermal accommodation with the surface prior to desorption. Interestingly, the J state populations, though colder, are also highly excited in a non-Boltzmann distribution, [$\langle E_{rot} \rangle$ = 1.0(1) kcal/mol], which indicates that a substantial fraction of molecules also directly scatter into the gas phase without rotationally equilibrating with the surface. Finally, nascent HF recoils from the liquid surface with excess translational energy, resulting in Doppler broadened line widths that increase systematically with internal HF excitation. The data are consistent with *microscopic branching* in HF-surface dynamics following the reactive event, with i) a direct reactive scattering (DRS) fraction of newly formed product molecules leaving the surface promptly and ii) a trapping desorption (TD) fraction that accommodates rotationally (though still not vibrationally) with the bulk liquid. Comparison with crossed molecular beam gas phase H atom abstraction processes in our group (such as F + ethane)[10] reveals a notably *hotter* HF vibrational distribution than observed at the gas-liquid

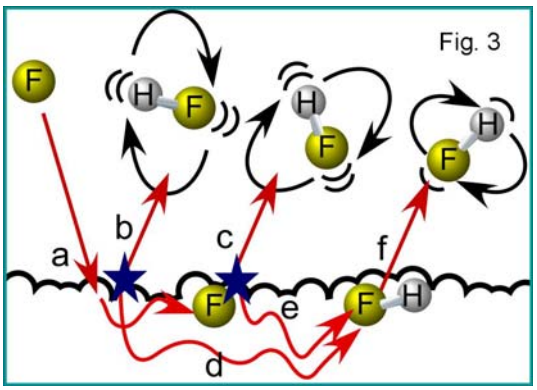


Fig. 3

interface, suggesting that the liquid acts as a partial but incomplete "heat sink" for vibrational energy flow on the time scale of the chemical reaction event.

D. 3D Quantum State Resolved Collision Dynamics at the Gas-Liquid Interface

A critical synergy over the past granting period has been harnessing theoretical molecular dynamics simulations in parallel with experiment (Fig. 4) in order to elucidate the underlying chemical physics. Specifically, large scale MD trajectory calculations have been performed for collisions of CO_2 with a model fluorinated self-assembled monolayer surface (F-SAMs), based on an explicit atom-atom interaction potential obtained from earlier theoretical studies with the Hase group.[3] Initial conditions for the simulations are chosen to match those in our experimental studies, i.e., with high-energy jet-cooled CO_2 molecules (E_{inc} = 10.6(8) kcal/mol, $\langle E_{rot} \rangle \approx 10\ cm^{-1}$) scattered from a 300 K perfluorinated liquid surface over a range of incident angles (θ_{inc} = 0º – 60º). The nascent CO_2 rotational distributions prove to be remarkably well-characterized by a simple two-temperature trapping-desorption (TD) and impulsive scattering (IS) model, with nearly quantitative agreement between experimental and theoretical column integrated densities. Furthermore, three-dimensional (3D) quantum state resolved flux maps for glancing incident angles ($\theta_{inc} \approx 60^o$) reveal broad, lobular distributions peaking strongly in the forward subspecular direction as $\cos^n(\theta_{scat} - \theta')$, with n ≈ 5.6(1.2) and θ' ≈ 49(2)º. As expected, the component of the scattered flux that proceeds by trapping desorption is equilibrated to the surface temperature. However, the quantitative success of a dual temperature characterization for rotation is consistent with a *broad distribution* of collision number and duration even for molecules recoiling in a nominally "impulsive scattering" channel, as further confirmed by detailed analysis of the trajectory statistics.

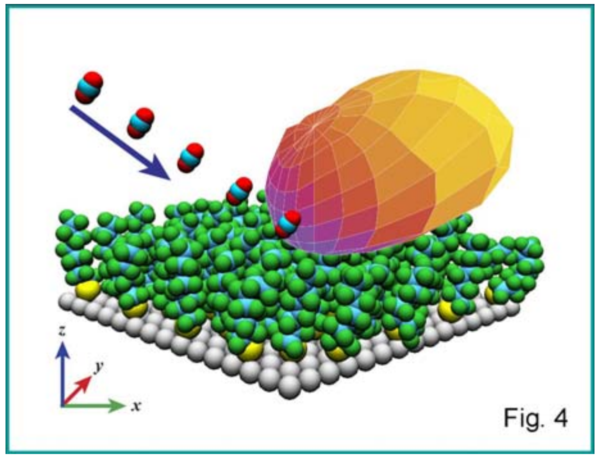


Fig. 4

E. Molecular Beam Reactive Scattering Dynamics via IR Direct Absorption

The quantum state resolved IR methods described above have also demonstrated extraordinary power in studying *reactive* scattering dynamics of F + $H_2O \rightarrow$ HF + OH under single-collision, crossed supersonic jet conditions (Fig. 5).[11] Nascent HF(v,J) rovibrational populations (v ≤ 2, J ≤ 17) at 5.4(1.3) kcal/mol are found to be highly inverted, with 75(2)% and 21(5)% of the observed HF product formed in v = 1 and 0, respectively. Small but finite branching [5(1)%] into the v = 2 manifold is observed, which is accessible only via the additional center of mass collision energy provided by the crossed jet collision geometry. Despite energy constraints associated with substantial *vibrational* excitation, the reaction dynamics also lead to *rotationally* hyperthermal HF, with populations observed up to near the energetic limit for each of the v = 0,1,2 vibrational manifolds. The trends in these nascent product rovibrational distributions support a strongly bent,

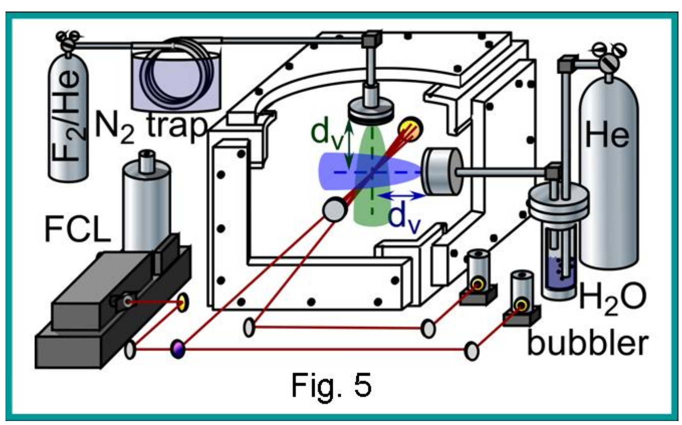


Fig. 5

early barrier transition state with long-range dipole-dipole interactions in the exit channel, in excellent agreement with high level MCSCF/MRCI surfaces calculated in our group.[12]

F. Non-Adiabatic Reaction Dynamics in Atom + Triatom Systems

Reactive collision dynamics in open shell systems offers even more sensitive methods for probing nascent quantum states of the radical product. For example, we have also explored crossed supersonic jet studies of $F + H_2O \rightarrow HF + OH(^2\Pi_{3/2}, {}^2\Pi_{1/2})$ under low density, single collision conditions at E_{com} = 6(2) kcal/mol, exploiting laser induced fluorescence (LIF) methods to yield rotational, vibrational, and spin-orbit state distributions in the nascent OH.[13] Of critical dynamical interest is the Wigner non-crossing rule, which predicts the lowest *adiabatic* reaction barriers on the ground and first excited electronic surfaces at $\Delta E \approx 4$ kcal/mol and $\Delta E \approx 25$ kcal/mol for formation of $OH(^2\Pi_{3/2})$ and $OH(^2\Pi_{1/2})$, respectively. In contrast, despite the fact that only reactions on the *ground state* potential are Born-Oppenheimer allowed at our experimental collision energy, both *ground and excited* spin-orbit OH products are observed in a substantial ($^2\Pi_{3/2} : {}^2\Pi_{1/2}$ = 69(1)% : 31(1)%) branching ratio. This indicates unambiguously the presence of strong *non-adiabatic surface hopping* interactions,[14-16] in agreement with previous results for $F + D_2O \rightarrow DF + OD$.[17] Interestingly, despite clear differences in the *rotational* distributions between $F + H_2O$ and $F + D_2O$ isotopic reactions, the overall *electronic* branching into spin-orbit manifolds is nearly identical for both OH and OD products. Furthermore, when plotted versus *total electronic + rotational* energy (Fig. 6), the nascent OH and OD populations each lie on single curves, with pronounced kinks in the Boltzmann plots suggestive of microscopic branching in the reaction dynamics. Such an equivalence of electronic and rotational energy release in the OH/OD products is consistent with nonadiabatic processes taking place in the immediate post transition state region rather than asymptotically in the exit channel.

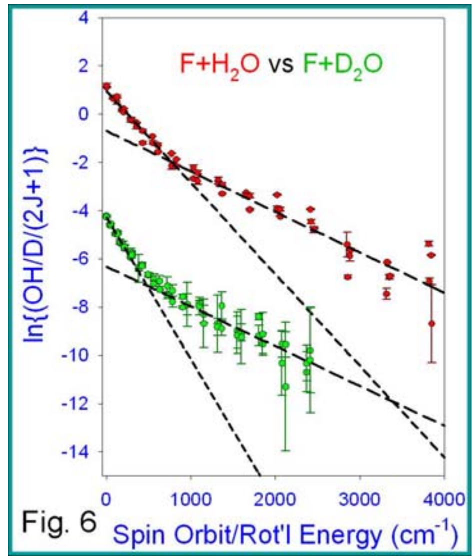


Fig. 6

G. IR Laser Polarization Studies of Stereodynamics at the Gas–Liquid Interface

By way of contrast with the isotropically averaged environment of bulk liquids, the gas-liquid interface offers a fascinating window into *non-isotropic* collision dynamics. Specifically, stereodynamics at the gas–liquid interface has been investigated by molecular beam scattering of CO_2 from liquid PFPE at E_{inc} = 10.6(8) kcal/mol, θ_{inc} = 60°, with internal quantum state populations and M_J distributions probed by high resolution, polarization modulated infrared laser spectroscopy.[4] Experimentally, polarization modulation of a single mode diode laser is combined with lock-in detection to measure circular/linear IR polarizance due to CO_2 scattering from the surface and probed over a series of final scattering angles. The differential absorption intensities are related through Fano-Macek theory to the three lowest multipole moments (A_0, A_{2+}, and O_{1-}) which describe collisionally

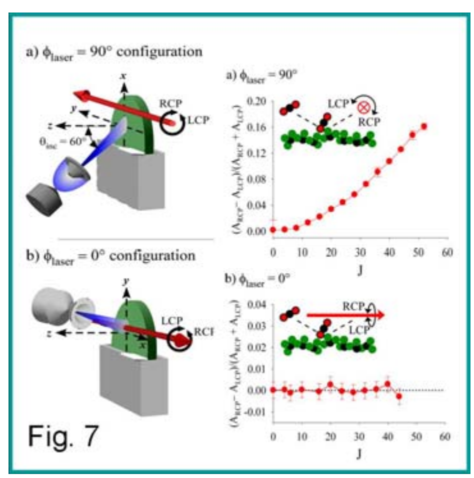
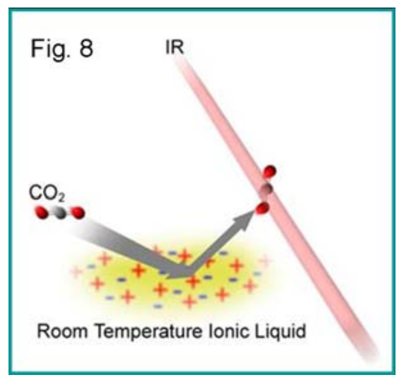


Fig. 7

induced orientation and alignment at the liquid surface.[18] The total scattering population reflects both trapping desorption (TD) and impulsive scattering (IS) components, with a strong *positive* anisotropy in the M_J distribution that indicates preferential CO_2 scattering from the surface with a *forward* (i.e., "top-spin") sense of end-over-end tumbling. Interestingly, the magnitude of the orientation/alignment parameters increases *monotonically from zero* as a function of final J state (Fig. 7a). This is consistent with the correspondence principle (i.e., J=0 can only be M_J =0) as well as a simple physical picture of greater torque on the projectile at the liquid interface resulting in both greater rotational excitation and alignment. Theoretical trajectory simulations provide 3D CO_2 flux and **J** state distributions scattering from fluorinated self-assembled monolayers (F-SAMs), which can be compared with experimental results as a function of final rotational state. Trends in the theoretical orientation/alignment moments are in remarkable agreement over the full range of J-states but with values consistently overpredicted by 2-fold, which provides clear evidence for a higher level of local ordering in F-SAMS vs. PFPE liquid interfaces.

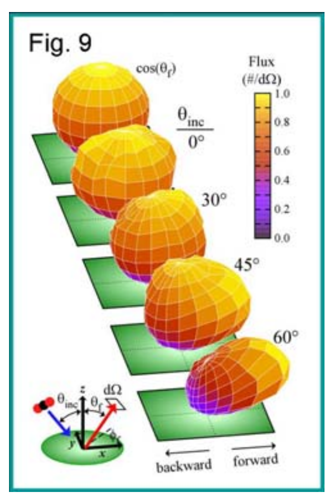
H. State Resolved Scattering at Room-Temperature Ionic Liquid-Vacuum Interfaces

Room-temperature ionic liquids represent a novel class of "green" solvents with nearly zero vapor pressure, high solubility for specific molecules, and therefore of keen industrial interest as possible carbon-sequestration and CO_2 scrubbing agents in natural gas reforming processes. Furthermore, due to their high charge density and electrical conductivity, RTILs are proving to be of considerable use in ionic thrusters for microsatellite propulsion and positioning. We have recently initiated state-resolved scattering studies (Fig. 8) of CO_2 from alkylimidazolium-based RTIL surfaces, containing either BF_4^- or Tf_2N^- anions, a direction which will be explored further in this granting period.[19] The scattered CO_2 exhibits a two-temperature rotational distribution, well described in the context of a trapping-desorption/impulsive-scattering (TD/IS) model. We find that the scattering dynamics for short alkyl chains are highly dependent upon the anion identity, implying that the anions are present at the interface and may play a critical role in the gas-liquid collisions. However, trends in the trapping-desorption fractions are in stark opposition with trends in the bulk Henry's Law solubility constants, clearly highlighting the critical role of *non-equilibrium* interfacial dynamics over *equilibrium* bulk solubility properties in these high-energy collisions.



I. High Resolution Dopplerimetry Scattering at the Gas – Liquid Interface

The high resolution ($\Delta\nu \approx 0.0001$ cm^{-1}) of the IR probe laser also provides an exceptionally detailed map of the quantum state specific recoil *vector velocities* in the gas-liquid scattering event. By way of example, full three dimensional (3D) translational distributions for quantum state-resolved scattering dynamics at the gas-liquid interface have been explored for experimental and theoretical studies of CO_2 + perfluorinated surfaces (Fig. 9).[2] Experimentally, high resolution absorption profiles are measured as a function of incident (θ_{inc}) and scattering (θ_{scat}) angles for CO_2 that has scattered from a 300 K PFPE surface with an incident energy of E_{inc} = 10.6(8) kcal/mol. Line shape analysis of the absorption profiles reveals *non-equilibrium* dynamics that are characterized by trapping-desorption (TD) and impulsive scattering (IS) components, with each channel characterized by an effective Doppler temperature that agrees surprisingly well with analysis based solely on rotational distributions. Molecular dynamics (MD) simulations of CO_2 + fluorinated self-assembled monolayer surface (F-SAMs) yield trajectories parsed by the scattering angle θ_{scat} and *J*, with the results corrected by rigorous flux-to-



density transformation and providing comparisons in remarkably quantitative agreement with experiment. 3D flux and velocity distributions obtained from MD simulations are also presented to illustrate the importance of in- and out-of-plane scattering. It is worth noting that such an experimental capability provides data for scattering into the "full 2π" solid angle, which is one of many powerful advantages of high resolution direct absorption laser methods.

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3) Brad Perkins (graduate student)
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Interactions/Transitions:
Invited talks during the2008-2011 granting period acknowledging AFOSR support:

“Bouncing Molecules from Liquids with Quantum State Resolution,” Departments of Chemistry and Chemical Biology, Harvard-MIT, Cambridge, MA, February 21, 2008.

“Searching for Simplicity: From Gas-Liquid Scattering to Single Molecule RNA Folding,” Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, March 6, 2008.

“Single Molecule Thermodynamics of RNA Folding,” Biophysics Supergroup, University of Colorado, Boulder, CO, March 10, 2008.

“The Physics of One: From Quantum Dot Blinking to Single Molecule RNA Folding,” National Institute of Standards and Technology Seminar Series, Boulder, CO, March 12, 2008.

“Searching for Simplicity: From Gas-Liquid Scattering to Single Molecule RNA Folding,” Crawford Lecture, Department of Chemistry, University of Minnesota, Minneapolis, MN, April 1, 2008

“Spectroscopy and Reaction Dynamics of Open Shell Species: A Quantum State Resolved Perspective,” Electronic Structure and Reaction Dynamics Symposium, 235th National ACS Meeting, April 6, 2008.

“From Jet Cooled Molecular Ions to Scattering at the Gas-Liquid Interface,” Molekülphysik Abteilung, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, May 9, 2008.

“State Resolved Collision Dynamics at the Gas-Liquid Interface,” Atomic and Molecular Interactions Gordon Conference, New London, NH, July 7, 2008.

“Polarization Studies of Quantum State Resolved Inelastic Energy Transfer and Stereodynamics at the Gas-Liquid Interface,” Stereodynamics of Chemical Reactions 2008, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, P. R. China, October 15, 2008.

“IR Laser Studies of Rovibrationally State-Resolved Reactive Scattering,” Frontiers in Physical Chemistry, Academia Sinica and National Taiwan University, Taipei, Taiwan, October 20, 2008.

“IR Laser Studies of Molecular Transients: Dynamical Insights Through High Resolution Spectroscopy,” Department of Chemistry, Kyushu University, ukuoka, Japan, October 29, 2008.

"Reactive and Inelastic Dynamics at the Gas-Liquid Interface with Quantum State Resolution," Gordon Research Conference on Molecular Energy Transfer,” Ventura, CA, January 21, 2009.

“Searching for Simplicity: From Collisions at Gas-Liquid Interfaces to Single Molecule RNA Folding,” Department of Chemistry, University of Indiana, Bloomington, IN, February 12, 2009.

“Searching for Simplicity: From Gas-Liquid Scattering to Single Molecule RNA Folding,” Department of Chemistry , Georgia Tech/Emory University, Atlanta, GA, March 2, 2009.

“Dynamics at Gas-Liquid Interfaces,” Physical Chemistry Chemical Physics Editorial Meeting, Barcelona, Spain, April 24, 2009.

“Bimolecular Collision Dynamics: An Overview,” Dynamics of Molecular Collisions, Snowbird, UT, July 6, 2009.

“Laser Studies of Jet Cooled Radicals: High Resolution Spectroscopy to Gas-Liquid Collision Dynamics,” 30th International Symposium on Free Radicals, Savonlinna, Finland, July 27, 2009.

“State-resolved reactive scattering: Gas-phase vs. gas-liquid dynamics,” 238th Meeting of the American Chemical Society, Washington, DC, August 17, 2009.

“State-resolved Dynamics at the Gas-Liquid Interface: A High Resolution Perspective,” Department of Molecular and Laser Physics, Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, The Netherlands, March April 2, 2010.

“State-Resolved Dynamics from Experimental and Theoretical Perspectives: How a Sabbatical Month with Joachim Changed my Life,” First Principles Quantum Chemistry 2010, Bad Herrenalb, Germany, April 16, 2010.

“Large Amplitude Motion and Roaming Dynamics: What Radicals May Have to Say at High Resolution,” Workshop on Roaming-Radical/Multiple-Mechanisms, Argonne National Laboratory and JILA, University of Colorado, May 7, 2010.

“High Resolution Spectroscopy and Dynamics: From Jet-Cooled Radicals to Gas-Liquid Interfaces,” 65th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, OH, June 23, 2010.

“State-Resolved Collision Dynamics and Spectroscopy at Gas-Liquid Interfaces,” Gordon Research Conference on Vibrational Spectroscopy, University of New England, Biddeford, Maine, August 2, 2010.

“From Combustion Radicals to Gas-Liquid Interfaces: Insights from High Resolution Laser Spectroscopy,” 21st International Conference on High Resolution Molecular Spectroscopy
Poznań, Poland, September 11, 2010.

“Large Amplitude Quantum Dynamics: A High Resolution Perspective on Unimolecular Rearrangement,” Anharmonic Vibrations of Molecules and Clusters: Experiment and Theory, Pacifichem 2010, Honolulu, HI, December 18, 2010.

“State-to-State Collision Dynamics: New Frontiers at the Gas-Liquid Interface,” Frontiers of State-to-State Dynamics, Pacifichem 2010, Honolulu, HI, December 19, 2010.

“In Search of Simplicity: From Spectroscopy of Radicals to Collisions at the Gas-Liquid Interface,” Department of Chemistry, University of Virginia, Charlottesville, VA, March 25, 2011.

“State-resolved Collision Dynamics at Interfaces: From Insulating Liquids to Molten Metals,” Chemical Reactions and Dynamics at Surfaces, 241st American Chemical Society, National Meeting, Anaheim, CA, March 27, 2011.

“Quantum State Resolved Velocity-Map Imaging Spectroscopy: A New Tool for Collision Dynamics at Gas/Self-Assembled Monolayer Interfaces,” Frontiers in Spectroscopy, Faraday Discussions 150, Basel, Switzerland, April 8, 2011.

“Quantum State Resolved Dynamics at the Gas-Liquid Interface,” Department of Chemistry, University of Washington, Seattle, WA, April 20, 2011.

“Searching for Simplicity: From Quantum State Resolved Collision Dynamics at the Gas-Liquid Interface to Single Molecule RNA Folding,” Department of Chemistry, University of Oregon, Eugene, OR, May 2, 2011.

“In Search of Simplicity: From IR Laser Spectroscopy of Combustion Radicals to Thermodynamics/Kinetics of Single Molecule RNA Folding,” 2010-2011 Frost Lecture, Department of Chemistry, Kingston, Ontario, Canada, May 13, 2011.

“Thermodynamics at the Single Molecule Level: RNA Folding in Laser Nanobathtubs,” Technische Universitaet Dresden, Dresden, Germany, June 10, 2011.

“Role of Multiple Exciton Generation and External Fields in Quantum Dot Blinking Dynamics,” Optical Probes 2011/Excited State Processes 2011, Santa Fe, New Mexico, June 21, 2011.

“Probing Non-Equilibrium Collision Dynamics at the Gas-Liquid Interface with Quantum State Resolution,” 2011 National Meeting, American Chemical Society Denver, CO, August 29, 2011.

“Energy Transfer Dynamics at the Gas-Liquid Interface: A Quantum State Resolved Perspective,” COMET 2011, Oxford University, Oxford, UK, September 15, 2011.

“Searching for Simplicity: From Collisions at Gas-Liquid Interfaces to Single Molecule RNA Folding,” Department of Chemistry, University of Pennsylvania, Philadelphia, PA, November 10, 2011.

“Watching Chemistry at the Single Molecule Level,” Frederick Kaufman Memorial Lecture Series, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, November 21, 2011.

“In Search of Simplicity: From Spectroscopy of Radicals to Collisions at the Gas-Liquid Interface,” Frederick Kaufman Memorial Lecture Series, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, November 22, 2011.

Consulting/Advisory Functions:

Editorial Board, Journal of Chemical Physics
Editorial Board, Journal of Physical Chemistry

Editorial Board, Molecular Physics
Editorial Board, Chemical Physicsl Letters
Advisory Board, Phys Chem Chem Phys

Inventions and Patent disclosures:
None

Honors, Awards or Fellowships received (2008-2011)
Presidential Rank Award, 2009
Fellow of the American Chemistry Society, 2010